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Length dependence of heat conduction in (an)harmonic chains with asymmetries or long range interparticle interactions

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HIGHLIGHTS

- Microscopic study of the heat flow.
- Changes on heat conduction due to graded structures.
- Nontrivial effects on thermal conductivity due to long range interactions.

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ABSTRACT

Considering an old and recurrent problem of nonequilibrium statistical physics, namely, the microscopic study of the heat flow, we investigate the effects on the heat conduction due the addition of graded structures or long range interactions in some usual models given by chains of oscillators. We show that the presence of these ingredients may considerably change the behavior of the heat flow with the system size, leading to new and unusual features: for example, the decay rate of the heat flow with the system length is increased in the presence of growing graded masses in a chain with local interactions; and we can observe, upon the inclusion of long range interparticle interactions, both the decline and the subsequent rise of the heat current in the same system by varying its length. Since our description is based on generic microscopic models, we expect to have results with some validity in real materials, and so, with practical application in the building of devices used to control and manipulate the heat flow.

1. Introduction

Heat transport in solids (and even in some liquids) is expected to obey Fourier's law, an old phenomenological law which states that the heat current is proportional to the temperature gradient: $\mathcal{F} = -\kappa \nabla T$ [1]. It means a diffusive transport, and gives the precise behavior of the heat flow with the system size: in a homogeneous bar of length N, submitted to a very small difference of temperature δT, $\mathcal{F} \sim -\kappa \delta T/N$. Although it is still missing a complete understanding of the necessary and sufficient conditions determining its validity, such law is observed in many real materials, and the famous parabolic

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heat equation, present in our textbooks of partial differential equations, is based on it. In the investigation of its microscopic mechanism, it is well known that Fourier's law does not hold in a fully harmonic system [2], but it is valid in chains with anharmonic on-site potentials. However, it is also well known, since the investigations following the seminal work of Fermi, Pasta and Ulam [3], that Fourier's law does not hold in one-dimensional momentum-conserving systems (with some exceptions, such as the rotator model [4]). That is, Fourier's law may be absent even in some intricate systems with a nonlinear dynamics. In such chains, with translational invariant interactions, exhaustive numerical simulations indicate that the heat flow decays with the system length as $1/N^{1-\alpha},\ \alpha > 0$, which means that the thermal conductivity diverges with length as N^{α} (so-called a superdiffusive behavior).

Several works have been devoted to the theme, most by means of numerical techniques or computer simulations due to the huge difficulty of the associated nonlinear dynamics [5]. In particular, the value of the exponent α has been recurrently investigated. According to the approach, different values of α are suggested: e.g. 1/3 [6], 2/5 [7] and 1/2 [8]. Recently, some works considering detailed numerical analysis of some translational invariant models indicate that the exponent α may change with the lattice length N. In Ref. [9], the authors claim that, in one-dimensional FPU-β and FPU-$\alpha\beta$ models, for some large values of N the exponent α observed is 1/3. However, for greater chains, the divergence of κ becomes faster and α increases to 2/5. A similar behavior, namely, changes in the thermal conductivity κ with the lattice length, is also reported in Ref. [10], for the same FPU-$\alpha\beta$ and one other model. In the mentioned work, the authors observe that, due to strong finite-size effects, the heat conduction obeys a Fourier-like law ($\alpha = 0$) in a wide range of lattice lengths, but, in yet longer lattice lengths, the thermal conductivity κ regains its power-law divergence, with $\alpha = 1/3$. Ultimately we cite Ref. [11], where the length dependence of heat conduction at different temperature regimes was investigated by considering a structural phase transition in a momentum conserving model.

To summarize, the study of the heat flow features starting from microscopic models, in particular, its behavior with the system size, is an old, recurrent and still important problem in nonequilibrium statistical physics, both for fundamental reasons as well as for practical applications: nowadays, with the advent of nanotechnology, new materials can be lithographically fabricated to present different properties, making possible the realization of devices to control and manipulate the heat flow, such as thermal diodes, and thermal gates [5].

In this work, we aim to unveil different behaviors and regimes of heat transport starting from usual models, given by harmonic and anharmonic chains of oscillators. Instead of investigating intricate and very particular systems, we search for the on-set of new properties in these basic models due the introduction of unusual features, precisely, of structures spread out over the system, such as asymmetries (graded structures) or long range interactions. By long range we mean polynomial decay (and so, here short range denotes exponential decay or compact support).

We emphasize the realizability of our results: the study of systems with long range interactions or graded structures is not a merely academic exercise. The role played by the interaction range is responsible for several phenomena and effects in microscopic and macroscopic physics, in electronic transport, in phase transitions, etc. [12]. Moreover, as already said, nowadays nanomaterials can be fabricated and manipulated to present different properties. An example of manipulated systems is given by magnets of nanodisks of Permalloy [13], exhaustively studied systems with interparticle interactions with polynomial decay $1/r_{i,j}^3$. We also stress that graded materials, i.e., inhomogeneous systems whose composition and/or structure change gradually in space, are abundant in nature, can also be manufactured, and have attracted great interest in many areas [14].

Thus, besides new theoretical knowledge, we believe that our results, obtained in these generic models, may provide hints for possible manipulation and construction of materials with different thermal conductivities.

2. Model and approach

We start from microscopic models recurrently used in the study of heat conduction in solids: chains of oscillators. Our approach holds for several different cases, as we describe ahead.

We take N classical oscillators in one-dimensional chains (for simplicity), with Hamiltonian

$$H = \sum_{j=1}^{N} \left(\frac{p_j^2}{2m_j} + \frac{M_j q_j^2}{2} + \sum_{\ell \neq j} \frac{J_{j\ell}}{2} q_j q_\ell + \lambda \mathcal{P}(q_j) \right), \tag{1}$$

where $M_j \geq 0$ is the pinning quadratic term; $J_{\ell j} = J_{j\ell}$ is the interparticle interaction; $\mathcal{P}$ is the anharmonic on-site potential: and so, $\lambda = 0$ for the specific harmonic case. The dynamics is given by the stochastic differential equations

$$\mathrm{d}q_j = (p_j/m_j)\mathrm{d}t, \qquad \mathrm{d}p_j = -\frac{\partial H}{\partial q_j}\mathrm{d}t - \zeta_j p_j \mathrm{d}t + \gamma_j^{1/2}\mathrm{d}B_j, \tag{2}$$

where B_j are independent Wiener processes; ζ_j is the coupling between site j and its reservoir (for the models with baths only at the boundaries, $\zeta_j = 0$ if j is an inner site); and $\gamma_j = 2\zeta_j m_j T_j$, where T_j is the temperature of the jth bath.

The harmonic version of this model ($\lambda = 0$) with a bath linked to each site was proposed long time ago in Ref. [15] (where homogeneous structures and nearest neighbor interaction were considered), and it is recurrently revisited, see e.g. Ref. [16]. Nevertheless, even in the case of quadratic potential solely, this model is a sort of an effective anharmonic